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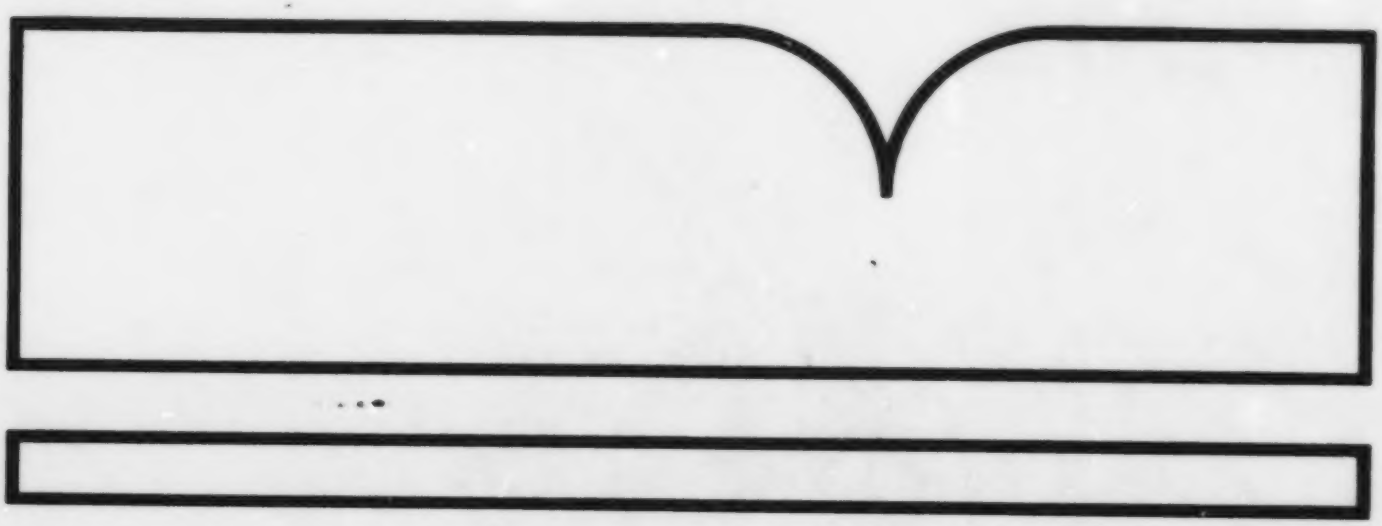

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USE OF LINEAR FREE ENERGY RELATIONSHIPS AND AN EVALUATIVE MODEL TO ASSESS THE FATE AND TRANSPORT OF PHTHALATE ESTERS IN THE AQUATIC ENVIRONMENT

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ABSTRACT -- Linear free energy relationships for selected phthalate esters were used to estimate the rate constants for hydroysis, biolysis, sediment-water partition coefficients, and biosorption required for modeling. The fate and transport behavior of dimethyl, diethyl, di-n-butyl, di-n-octyl, and di-(2-ethylhexyl) phthalate esters were assessed by use of an evaluative model, the Exposure Analysis Modeling System (EXAMS). Four EXAMS environments were defined: a pond, an oligotrophic lake, a eutrophic lake, and a river using environmental parameters representative of the Southeastern United States. Results suggest that higher molecular weight esters are not significantly transformed and that export from the ecosystem is the dominant process.

INTRODUCTION

Phthalate esters are a widespread contaminant of freshwater and saltwater aquatic environments (1,2). Although manufactured in large volumes (more than 10^5 tonnes in 1976), few reports on the fate and transport of these chemicals have been published (3). The phthalates are susceptible to alkaline hydrolysis, with theoretical half-lives at pH 8 and 30°C ranging from 4 months to 100 years (4). The overall significance of this hydrolytic degradation of phthalates in aquatic environments cannot be fully assessed, however, from hydrolysis rate constants alone. The net degradation of chemicals in the environment depends both on the physical and chemical properties of the compound (e.g., sorption and reaction pathways) and on the reaction conditions (e.g., pH, light intensities) and transport patterns imposed by the environment itself.

One instructive technique for amalgamating the properties of chemicals and environments, and thereby predicting the behavior of chemicals in the environment, lies in the use of evaluative models (5,6). Implementation of the models on computers provides a convenient tool for projecting the laboratory chemistry of a compound into a fuller environmental context and for estimating the degree to which any particular degradation pathway will be effective in mitigating environmental pollution. Models and computer programs require an irreducible minimum of quantitative information for even the most tentative of estimates, however, and the experimental studies needed to provided this minimum data base for the phthalate esters have not as yet been performed.

When experimental data are lacking, some of the chemical and physical information needed for evaluative purposes can be estimated from structure-reactivity relationships (7). Linear free energy relationships (LFERs) were employed in this study to augment the available data on phthalate esters. The full data base was then coupled to a computerized evaluative model in order to assess fate and transport of selected phthalate esters in simulated aquatic environments.

Five phthalate esters were considered in this study: dimethylphthalate (DMP), diethylphthalate (DEP), di-n-butylphthalate (DNBP), di-n-octylphthalate (DNOP), and di-(2-ethylhexyl)phthalate (DEHP). These esters were selected because they are produced in large quantities and represent a cross-section of chemical reactivities and physical properties within the class.

RESULTS

EVALUATIVE MODEL

Simulation studies of the behavior of these phthalate esters in the aquatic environment were executed using the Exposure Analysis Modeling System (EXAMS) (8). A multicompartment kinetic model, EXAMS synthesizes fate and transport processes under a specified set of environmental conditions. The model employs mathematical descriptions of physical, chemical, and biological fate processes derived from laboratory studies. The EXAMS computer code allows a user to select particular process models from a number of alternatives, by controlling the structure of the input data. This study was designed to provide some insight into the range of possible behaviors of the phthalate esters over the chemical class and over a range of simple environmental differences. Consequently, the environments were defined in terms of spatially homogeneous water-bodies having relatively simple transport regimes.

Four EXAMS environments were defined and coupled to the data base describing the chemistry of the phthalate esters. These environments included: a 1 hectare (ha) pond with a 30-day detention time; an oligotrophic (weakly stratified) lake and an eutrophic (stratified) lake, each having a 200-day total detention time and an area of 35 ha; and a river segment of 100 m in width and 3 km in length with a detention time of 1 hour. The environmental parameters that determine the reaction conditions in the water bodies were chosen to represent usual summertime values in the Southeastern United States. Some of the chemical, physical, and biological characteristics of the EXAMS ecosystems are given in Table 1; other parameters not summarized in this table are detailed below.

Table 1. Physical, Chemical, and Biological Characteristics of Ecosystems Used in the EXAMS Model

	River (3 km)	Pond	Eutrophic lake	Oligotrophic lake
Volume (m^3)	$9x10^8$	$2x10^4$	$8x10^9$	$8x10^9$
Water Input (m^3/hr)	$9x10^5$	$2.8x10^1$	$1.1x10^3$	$1.1x10^3$
Suspended Sediment (mg/l)	100	30	50	10
pH	7.0	8.0	8.0	6.0
Bacterial Population (water) (cells/ml)	$1x10^3$	$1x10^3$	$1x10^5$	$1x10^2$
Bacterial Population (sediment) (cells/100g dry weight)	$1x10^8$	$1x10^8$	$1x10^{10}$	$1x10^7$
Sediment Organic Carbon (%)	1	4	4	1

The zenith light extinction coefficient was taken as 3.0 m^{-1} for all systems except the oligotrophic lake (0.3 m^{-1}), and the light distribution function (ratio of optical path to depth) was taken as 1.19 in all cases. EXAMS then computed the fractional reduction in photolysis rates resulting from light absorption in the water column. Bottom sediments in all systems had a bulk density of 1.85 g/cm^3, a water content of 150%, and an active depth of 5 cm. The benthic residence time for equilibration of the sediments with the overlying water was taken as 75 days for all systems except the river (10 days). Phthalate esters sorbed to suspended or benthic sediments were assumed to be "protected" from transformation processes. The concentration of free-radical oxidants was taken as 10^{-9} M in the water column of all systems and assumed to be negligible (zero) in bottom sediments. For volatilization, a wind speed of 2 m/s at 10 cm height was used for all systems. [This value is equivalent to a vapor phase transfer coefficient (piston velocity for water vapor) of 2291 cm/hr.] Reaeration rates, selected from Metcalf & Eddy (9), were 0.0072 hr^{-1} for the ponds, 0.012 hr^{-1} for the lakes, and 0.0168 hr^{-1} for the river. Volatilization of the phthalate esters was computed by a two-film method (8). The eddy dispersion coefficient for mixing across the thermocline in the eutrophic lake was taken as 0.08 m^2/hr (10). This value resulted in a hypolimnetic residence time of 52 days; the eddy dispersion coefficient for the oligotrophic (weakly stratified) lake was chosen to give a hypolimnetic residence time of 10 days.

USE OF LFERs

In the absence of experimental values, four separate LFERs were used to estimate the necessary constants for input into the EXAMS model in the assessment of these selected phthalate esters.

Hydrolysis rate constants

Recently, Wolfe and coworkers (4) established a LFER for the alkaline hydrolysis of phthalate esters (k_{OH}) that is described by the following linear equation.

$$\log k_{OH} = 4.59\,\sigma^* + 1.52\,E_s - 1.02 \qquad (1)$$

Using equation 1 and tabulated values of σ^* and E_s (11) for other alkyl groups, it is possible to estimate hydrolysis rate constants for other esters. The estimated value for DNOP is included in Table 2 along with the experimentally determined values previously reported (4).

Microbial degradation rate constants

Microbial rate constants (k_b, 1 org^{-1} hr^{-1}) (7,12,13) for selected organic compounds have been correlated with alkaline hydrolysis rate constants (k_{OH}, M^{-1} sec^{-1}) and the octanol/water partition coefficient (K_{ow}) (13). The correlation for four phthalate esters is described by

$$\log k_b = 2.1 \pm 0.4 \log k_{OH} - 6 \pm 1 \qquad (r^2 = 0.933) \qquad (2)$$

The microbial degradation rate constant (k_b) for DMP was been calculated using equation 2 and is given in Table 2 along with the experimentally determined values of k_b for the other esters (14).

Sediment/water partition coefficients

Several different correlations permit the estimation of sediment-water partition coefficients (15,16,17). The two used in this study are the relationships between the sediment-organic carbon content (K_{OC}) and either the water solubility (S) or the octanol-water partition coefficient (K_{ow}). An empirical relationship for estimating K_{OC} values with water solubility has been established by Karickhoff *et al.* (15) for ten compounds and extended to 22 compounds by Hassett and co-workers (17) as given by equation 3.

$$\log K_{OC} = -0.60 \pm 0.38 \log S + 1.21 \pm 0.22 \qquad (r^2 = 0.927) \qquad (3)$$

where S is the water solubility in moles/L. Although such a relationship should be adequate for organic liquids (12), care should be taken to insure that crystal lattice energies that can cause large deviation are taken into account in the case of solids.

The correlation of K_{OC} with K_{OW} (15,17) overcomes crystal lattice effects and is applicable to both solids and liquids (equation 4).

$$\log K_{OC} = 1.00 \log K_{OW} - 0.317 \qquad (r^2 = 0.983) \qquad (4)$$

If values of K_{OW} are not available, they too can be estimated. For example, a correlation was demonstrated using data for compounds that exist as liquids at room temperature and is given by equation 5,

$$\log K_{OW} = -0.65 \log S + 0.889 \qquad (r^2 = 0.874) \qquad (5)$$

where S is the molal water solubility (18). Using the measured water solubility for DEHP, the estimated K_{OC} value obtained using equations 5 and 4 is 4.80, which is in good agreement with the value of 4.55 obtained with equation 3. Other estimation methods for K_{OC} are available, such as the liquid chromatographic technique of Veith (19) or the substituent constants calculations described by Leo and co-workers (20).

Biosorption constants

A LFER between biosorption (K_B) for bacteria and the octanol/water partition coefficient (K_{OW}) was established for 14 compounds by Baughman and Paris (21). They reported the linear relation given by equation 6:

$$\log K_B = -0.907 \log K_{OW} - 0.361 \qquad (r^2 = 0.954) \qquad (6)$$

This equation, along with the calculated values of K_{OW} (equation 5) for the esters, was used to estimate the values of K_B reported in Table 2 for the five phthalate esters considered in this study.

CHEMICAL AND PHYSICAL PROPERTIES

The relevant properties of the phthalate esters are summarized in Table 2. The second-order acid-catalyzed hydrolysis rate constant (k_H) used for all five esters is an assumed value; neutral hydrolysis (k_{H_2O}) is not a detectable transformation pathway for these esters (4). The alkaline hydrolysis rate constant (k_{OH}) for DNOP was estimated from equation 5; the balance of the values are from Wolfe *et al.* (4). The (near-surface) rate constant for direct photolysis (k_d) of the phthalates is an estimate of its maximum value obtained by analysis of a solution of DMP in a natural water sample exposed to sunlight for one week (R. G. Zepp, oral communication, 1980). The free radical oxidation rate constants (k_{OX}) given in Table 2 were estimated based on average values reported for primary, secondary, and tertiary alkyl groups with peroxy radicals (22). Henry's Law constants (H) were obtained using measured water solubilities (4; Table 2) and vapor pressures (23) extrapolated to 25°C.

SIMULATION

Phthalate loadings into the environments were modeled by assuming that waters entering the system were contaminated at a level of 0.1 ppm. The EXAMS program then algebraically computed the steady-state behavior of the chemicals and, by numerical integration, the dissipation of phthalates from the system upon cessation of the external loads. The results of these simulations are summarized in Table 3 and Table 4.

Steady-state attenuation of these water-borne loadings was least in the unimpeded river system (Table 3). The percentage reduction of the load did

Table 2. Constants Used in the EXAMS Model for Assessment of the Fate and Transport of Five Phthalate Esters.[a]

	DMP	DEP	DNBP	DNOP	DEHP
k_H, $M^{-1}hr^{-1}$	0.04	0.04	0.04	0.04	0.04
k_{H_2}, hr^{-1}	--	--	--	--	--
k_{OH}, $M^{-1}hr^{-1}$	2.5×10^2	7.9×10^1	3.8×10^1	5.9×10^1	4.0×10^{-1}
k_d, hr^{-1}	2×10^{-4}	2×10^{-4}	2×10^{-4}	2×10^{-4}	2×10^{-4}
k_B, ml $org^{-1}hr^{-1}$	5.2×10^{-6}	3.2×10^{-9}	2.9×10^{-8}	3.1×10^{-10}	4.2×10^{-12}
k_{ox}, M sec^{-1}	18	18	18	18	18
H atm m^3/mole	1.1×10^{-6}	2.0×10^{-8}	1.3×10^{-6}	5.5×10^{-6}	4.4×10^{-7}
K_B	2.6×10^1	7.3×10^1	8.0×10^3	2.9×10^3	8.9×10^3
K_{oc}	1.6×10^2	4.5×10^2	6.4×10^3	1.9×10^4	5.7×10^4
S, mg/l	4.3×10^3	8.9×10^2	1.3×10^1	3.0	4.0×10^{-1}

[a]Physical and chemical constants defined in the text.

Table 3. Summary of Results of Computer Simulation of the Fate and Transport of Five Phthalate Esters in Four Aquatic Environments[a].

Compound	Ecosystem	Load Reduction (%)	Accumulation Factor (Days)	Distribution (%) Water Column	Bottom Sediment	Recovery Time
DMP	River	0.55	0.04	99.99	0.01	3 hr
	Pond	80.5	5.8	99.98	0.02	20 day
	Eutrophic lake	100.0	0.08	100.0	0.0	6.7 hr
	Oligotrophic lake	73.2	52.0	100.0	0.0	184 day
DEP	River	0.01	0.05	91.8	8.2	67 hr
	Pond	9.9	39.0	69.7	30.3	7 mo
	Eutrophic lake	62.4	65.0	99.8	0.2	8 mo
	Oligotrophic lake	14.8	174.0	98.3	1.7	20 mo
DNBP	River	0.07	0.09	45.7	54.3	18 day
	Pond	42.4	130.0	13.3	86.7	19 mo
	Eutrophic lake	92.3	11.7	96.4	3.6	40 day
	Oligotrophic lake	24.7	186.0	81.0	19.0	23 mo
DNOP	River	0.04	0.20	20.7	79.3	30 day
	Pond	27.4	521.0	4.2	95.8	67 mo
	Eutrophic lake	51.0	316.0	28.3	71.7	47 mo
	Oligotrophic lake	33.3	235.0	57.2	42.8	32 mo
DEHP	River	0.0	0.50	8.3	91.7	35 day
	Pond	4.8	1910.0	1.5	98.5	19 yr
	Eutrophic lake	11.4	1564.0	11.2	88.8	19 yr
	Oligotrophic lake	16.0	544.0	31.0	69.0	6 yr

[a]All results expressed in terms independent of the magnitude of the input loadings, in order to facilitate comparisons among esters and among ecosystems.

not exceed 0.6% for any of the esters, thus, better than 99% of the river loadings were simply transmitted down stream in all cases. Appreciable losses were predicted, as expected, in the systems with longer detention times (ponds and lakes). The observed load reduction was not a simple function of detention time; however, because in some instances (DMP, DNBP), the pond system (30-day residence time) removed more of the load than did the oligotrophic lake (200-day residence time).

The magnitude of contamination of these ecosystems by the phthalate esters was expressed in terms of an accumulation factor, i.e., a multiplier on the daily mass loadings (e.g., kg/day) that would yield the total mass (e.g., kg) ultimately residing in the system at steady-state (Table 3). Both rapid flushing (rivers) and substantial degradation of the esters was shown to be effective in limiting the degree of contamination. For example, load attenuation was forecast to be 100% and 92.3% in the eutrophic lake for DMP and DNBP, respectively, resulting in the smallest (non-riverine) accumulation factors (0.08 and 11.7) observed (Table 3). The tendency to accumulate was also dependent, however, on the affinity of the ester for bottom sediments. Increases in K_{OC} within the ester series (Table 1) generally resulted in concomitant increases in the proportion of the contamination that resided in bottom sediments (Table 3). For example, the largest accumulation factor (1910.0) was forecast for DEHP in the pond ecosystem, where less than 5% of the load was degraded and 98.5% of the contaminant occurred in the benthic sediments.

Recovery times for the contaminated ecosystems were estimated as five pseudo-first-order half-lives computed from the EXAMS numerical simulations. Separate half-lives were computed for the benthic sediment and water-borne sectors of the ecosystems, and the pseudo-first-order system half-life was weighted according to the distribution of the esters between the water column and the bottom sediments (Table 3). The recovery time was generally correlated with the size of the accumulation factor, reaching 19 years for DEHP contamination of the pond and eutrophic lake ecosystems.

The computed relative effects of hydrolysis, photolysis, biolysis, and volatilization of the phthalate esters on total attenuation of the input loadings to each ecosystem are presented in Table 4. Oxidation of the esters was predicted to be negligable (0.01% of the load or less) in all cases, and was omitted from the table. Biological degradation was the dominant transformation process in most instances. Photolysis, although slow, was forecast to be the primary breakdown process in the oligotrophic lake for all the esters except DMP, and in these instances accounted for 10 to 15% of the loadings at steady-state. DNOP was the most volatile ester, with predicted volatilization losses of about 20% of inputs in the systems that had appreciable detention times. Of the other esters, only DNBP was predicted to have any substantial (relative) tendency to volatilize, and that was restricted to systems that had relatively slight biolysis or flushing (i.e., the pond and the oligotrophic lake). Hydrolysis was generally too slow to compete with biolysis, although some exceptions (e.g., DEP and DNOP in the pond system) did occur.

DISCUSSION

The results of these evaluative simulations indicate that few universal generalizations apply to the phthalate esters as a class. For example, the structural differences between DMP and DEHP offer a contrast between a compound (DMP) that shows little tendency to be captured by bottom sediments, is rapidly degraded and exported from contaminated ecosystems, and exhibit minor accumulations within the system, versus a compound (DEHP) that accumulates significantly, is removed slowly from contaminated systems, and even under extreme reaction conditions tends to contaminate further environments downstream of the original receptor system. The structural isomers DNOP and DEHP are particularly instructive: volatilization from ponds and lakes accounts for about 20% of loadings of DNOP, but only 2% of DEHP loadings (Table 3); the Henry's Law constants for these isomers (Table 2) show a similar order-of-magnitude difference.

The significance and effective rate of each transformation pathway is also strongly affected by environmental conditions and by interactions among parameters. For example, the theoretical hydrolysis half-lives of DMP and DEHP at pH 8 and 30°C are 4 months and 100 years, respectively (4). The half-life for hydrolytic degradation (alone) in the eutrophic lake ecosystem at steady-state was indeed 4 months for DMP, but increased from 100 to 2000 years for DEHP, primarily as a consequence of capture of the ester by benthic sediments. In the oligotrophic lake, with its lower pH, hydrolytic transformations would require 31 years to cleanse the system of DMP (100 times slower than in the eutrophic lake), and 6000 years for DEHP. The decrease in the hydrolysis rate of DEHP between the eutrophic and oligotrophic lakes amounted to only a factor of 3, rather than the factor of 100 suggested by the change in pH. Because the oligotrophic lake sediment contained only 1% organic carbon (Table 1), less of the DEHP was captured by sediments and thus the compound was more available to hydrolytic decomposition.

Table 4. Transformation and Volatilization of Phthalate Esters in Four Aquatic Systems,Reported as the Percent of the Load That is Lost via Each Process at Steady-State. The Residual (Difference of the Sum from 100%) is Water-Borne Export.

Compound	Ecosystem	Hydrolysis	Photolysis	Biolysis	Volatilization
DMP	River	0.0	0.0	0.5	0.0
	Pond	3.5	0.4	74.5	2.2
	Eutrophic lake	0.1	0.0	99.9	0.0
	Oligotrophic lake	0.3	4.6	65.6	2.7
DEP	River	0.0	0.0	0.0	0.0
	Pond	2.8	1.8	5.1	0.2
	Eutrophic lake	6.7	0.7	55.0	0.1
	Oligotrophic lake	0.2	13.9	0.6	0.1
DNBP	River	0.0	0.0	0.1	0.0
	Pond	3.3	1.2	31.8	6.2
	Eutrophic lake	2.1	0.2	89.1	0.9
	Oligotrophic lake	0.3	12.3	4.9	7.2
DNOP	River	0.0	0.0	0.0	0.0
	Pond	1.4	1.4	0.5	24.0
	Eutrophic lake	5.6	0.8	28.6	16.0
	Oligotrophic lake	0.1	11.0	0.0	22.2
DEHP	River	0.0	0.0	0.0	0.0
	Pond	0.0	1.8	0.1	2.8
	Eutrophic lake	0.2	1.4	7.7	2.2
	Oligotrophic lake	0.0	13.7	0.0	2.3

CONCLUSIONS

The establishment of linear free energy relationships is a useful and convenient method for extending the existing data bases on the transport and transformation of environmental pollutants. These data are used in an evaluative model to assess the fate and transport of selected phthalate esters in simulated aquatic environments. The results of these simulations indicate that hydrolysis, biolysis, photolysis, volatilization, and export can all be competing processes depending on the properties of the ester and the ecosystem. In general, the higher molecular weight esters will probably not undergo significant transformation; and export from the ecosystem, although often slow, is forecast to be the dominant process.

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